Title: Rapid and Reliable Computational Markers for Predicting Daily Smoking Behavior and Smoking Cessation Treatment Outcomes

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Structured abstract

Importance: Nicotine addiction is a complex disorder shaped by factors such as craving, mood, and neurocognitive processes. While ecological momentary assessment (EMA) provides a real-time method for capturing dynamic changes in behavior, traditional tasks and surveys are often too lengthy and demanding for repeated use in clinical settings. Integrating EMA with computational approaches offers a promising solution to predict smoking behavior dynamically while addressing the practical limitations of conventional assays, paving the way for more effective and scalable interventions.
Objective: To evaluate the predictive value of computational markers derived from decision-making tasks and ecological momentary assessment (EMA) data for short-term (daily smoking behavior) and long-term (cessation success) outcomes, and to assess the timing and amount of data collection needed for prediction.
Design, setting, and participants: 79 daily smokers (mean age 25.64 years, 83% male) took part in a longitudinal experimental study involving EMA surveys of psychological states and decision-making tasks, delivered daily via a smartphone app, while undergoing a 5–6 week smoking cessation program. Using a machine-learning methodology (adaptive design optimization, ADO) to effectively generate task variables, we estimated computational markers from just 20 to 30 trials per day, reducing task length and participants burden.
Results: A time-lagged model incorporating both computational markers and self-reported daily psychological states provided the most accurate prediction of next-day smoking behavior. Higher levels of craving, depression, and ambiguity tolerance in decision-making on the previous day were significantly predictive of increased smoking amount the following day. Smoking cessation status at the end of treatment was most strongly predicted by lower discounting rates, reduced craving and stress, a longer smoking history, and greater engagement in treatment (AUC = 0.76). Notably, models based on data collected during the first week of follow-up, either on the decision-making tasks (AUC = 0.74) or psychological variables (AUC = 0.73), demonstrated comparable predictive accuracy for end-of-treatment smoking cessation.
Conclusions and relevance: Combining computational markers with EMA data offers a dynamic and efficient approach for predicting smoking behavior and cessation success and holds promise for clinical applications.

Key points

Question: Can computational markers from decision-making tasks combined with ecological momentary assessment (EMA) data accurately predict daily smoking behavior and cessation outcomes, and how does the timing and amount of data collection affect prediction?

Findings: This longitudinal study examined computational markers and psychological variables in daily smokers during a cessation program. Increased ambiguity tolerance, craving, and depression predicted next-day smoking, while lower discounting rates and reduced craving and stress in the first week were linked to successful cessation. Early data (first week) showed comparable accuracy in preidcting end-of-treatment cessation.

Meaning: Integrating computational markers with EMA data provides a dynamic and efficient method for predicting smoking behavior and cessation outcomes, offering significant potential for scalable clinical applications.

Introduction

Nicotine Use Disorder (NUD) is a major cause of morbidity and mortality worldwide[1]. Despite availability of various smoking cessation treatments, over two-thirds of smokers relapse within a year of a quit attempt[2,3]. The high smoking relapse rate emphasizes the need for identifying reliable predictors of successful cessation, particularly ones that smokers can integrate into their daily lives. Previous research has identified demographic, motivational[4], and environmental factors[5,6], as well as stress, negative affect[7,8] nicotine dependence[8,9] and nicotine craving[10,11] as barriers to maintaining abstinence. Recently, interest has grown in identifying cognitive "computational markers" that predict clinical outcomes. These markers, which are parameters derived from fitting mathematical models to cognitive tasks like risk and delay discounting[12,13], have proven useful in understanding neurocognitive mechanisms of a range of psychiatric conditions[12,14–18]. Such markers can enhance both clinical prediction and mechanistic insight into substance use disorders[19,20], including smoking cessation[21–23]. However, much of this research remains cross-sectional, despite addiction recovery being both dynamic and individualistic[12,13,19,20–23].

Ecological momentary assessment (EMA) methods have been increasingly used to capture dynamic, within-person variations in psychological states (i.e., mood, craving, and stress) in naturalistic settings[7,24,25]. While EMA has shown promise in addiction research[26–28], particularly for modeling temporal variations of self-reported psychological states with clinical utility[29,30], capturing similar dynamics in task-based cognitive markers remains a challenge[26–28,29,30].

The reasons for these failures may stem from two factors: First, traditional decision-making tasks are often lengthy and repetitive, reducing participant motivation and data quality, particularly in clinical populations[31]. Second, no previous study to our knowledge has successfully combined self-reported surveys and computational markers on a daily and longitudinal basis to predict smoking behavior. Such densely sampled data could capture finer temporal dynamics of factors associated with smoking cessation or relapse, providing ecologically valid and robust insights into the cognitive processes underlying addiction, as suggested in other substances[28]. Identifying critical moments and individual-specific decision patterns can guide real-time, personalized interventions tailored to individual trajectories, enhancing treatment effectiveness and long-term cessation success.

To overcome these limitations, we conducted a longitudinal study of cigarette smokers who completed two decision-making tasks (delay discounting and risk-taking) daily, alongside self-reported psychological states three times a day via a smartphone app for 5-6 weeks during a smoking cessation treatment (**Figure 1A**). We adapted two well-established tasks previously linked to drug reuse in laboratory-based studies: the delay discounting task[32], which measures choice impulsivity[33–35], and the choice under risk and ambiguity (CRA) tasks[36], which assesses risk and ambiguity-aversion[19]. We used the adaptive design optimization (ADO[37]) methodology—a machine learning (ML) algorithm based on Bayesian framework that selects the most informative stimulus combinations in real-time—to shorten the tasks delivery to just a few minutes of trials, thereby reducing participant fatigue and boredom. Even with fewer trials, ADO shows superior reliability and precision of behavioral parameter estimation than non-ADO methods[38,39].

We focused on two main objectives: first, we aimed to identify computational and psychological markers predictive of short-term (daily smoking behavior) and long-term

outcomes (abstinence at treatment completion). Second, we aimed to test the efficiency of ADO-powered computational markers in predicting the clinical outcome, specifically by examining the minimum amount of data required for prediction. These goals are particularly beneficial to achieve because identifying daily predictors of smoking behavior highlights the potential for adjusting treatment plans dynamically to improve outcomes, and predicting longer-term abstinence supports treatment selection and participant stratification, which offers valuable insights for individualized prognoses. Our results show that distinct computational markers predict short-term and post-treatment smoking behavior. Further, we demonstrate the usefulness of these markers for monitoring smoking behavior, with just one week of data being sufficient for making reliable predictions about cessation likelihood at the end of treatment.

Materials and Methods

Participants

We recruited daily smokers (N=143) who actively participated in a smoking cessation clinic (**Figure 1A**). The medication-assisted clinic included a weekly visit for prescription (i.e., varenicline or bupropion), nicotine replacement therapy (NRT; gum, candy, or patch) as needed, and a medical counseling session with a clinician for 5 to 6 weeks. Participants underwent a screening session to be decided if they met the following criteria: (1) smoked more than five cigarettes a day for the past year, (2) had no current or past psychiatric disorder diagnoses other than NUD, as assessed by the Structured Clinical Interview for DSM-5 Disorders: Clinical version (SCID-5)[40], (3) and urine drug screening (for stimulants, opioids, and cannabis) and a breath test (for alcohol), and (4) abstained from smoking cigarettes for 8 hours before the visits, confirmed with exhaled carbon monoxide (CO) measured. Ten participants were excluded after completing a screening session and 25 participants dropped out of the study, leaving a total of 108 participants with available data (**Figure S1**).

During the clinic attendance period, participants were asked to fill out surveys (see **Measures** below for the list of surveys) and complete the delay discounting and CRA tasks dialy via the smartphone application (**Figure 1B**). Participants were compensated with a financial bonus in accordance with their app participation (see **Supplementary materials**-Participants). Participants who completed fewer than 14 days (N=19) of surveys and/or tasks or had no participation in the first week (N=10) were excluded from the final analysis. Therefore, a total of 79 participants were included in the final analysis. All procedures were approved by the Institutional Review Board of Seoul National University.

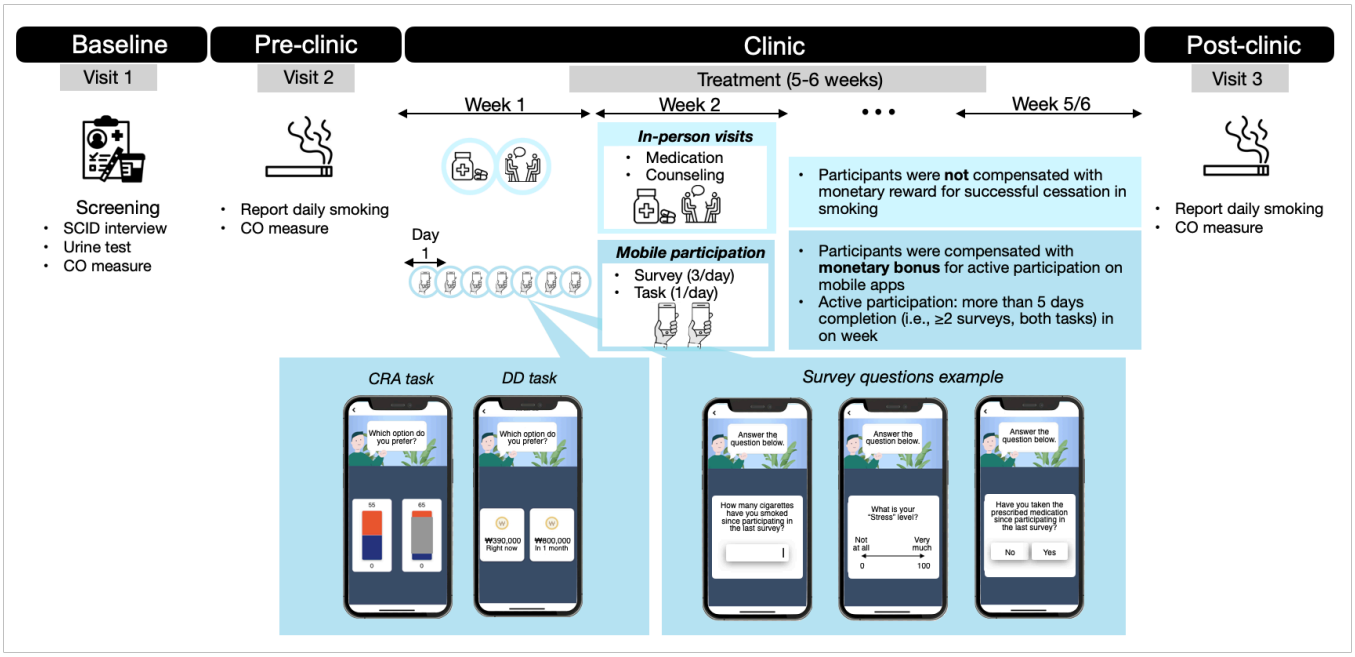

Figure 1. Study timeline and procedures. Data were collected from March 2019 to December 2022. Participants who passed the screening procedures during an initial lab visit made an additional two visits to the lab. During treatment, participants attended weekly in-person medication prescribing and counseling sessions at a unversity health center and participated in daily EMA surveys and behavioral tasks. On the bottom panel are sample screenshots of daily tasks and survey questions: CRA task (Choice under risk and ambiguity), DD task (Delay discounting).

Measures

Psychological state surveys and self-reported smoking

The app notified participants three times daily (9am, 2pm, 7pm) to rate their psychological state using a 0-100 scale (mood, stress, depression, anxiety, craving to smoke). They complete the surveys within three hours of notification, reporting cigarette consumption and doses of medication/NRT since the last response.

During pre- and post-clinic visits, participants reported their average daily cigarette use over the past week in four categories (0, ≤5, >5 but <10, and ≥10). They also completed questionnaires on nicotine dependence (Fagerström test for nicotine dependence, FTND; Cigarette Dependence Scale, CDS-12) and craving (Questionnaire on Smoking Urges, QSU-Brief), which are significant factors in determining smoking cessation.

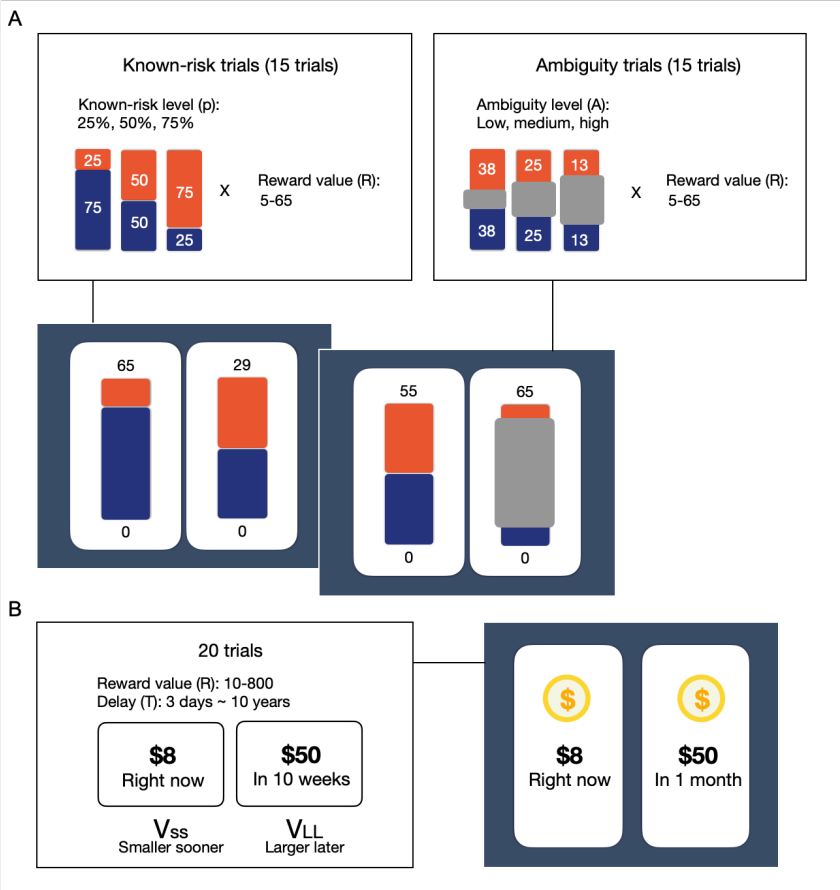

Figure 2. ADO-powered decision making tasks. (A) Choice under Risk and Ambiguity task. There are two types (known-risk and ambiguous) of trials, where participants choose between two options (one with the fixed 50% probability of winning a non-zero reward amount vs. one varying in probability of reward). **(B)** Delay discounting task. Participants chose between two options (larger but later reward vs. smaller but sooner reward). Note that dollar signs were used here to aid understanding, but participants were presented with Korean won on a similar scale.

Decision-making tasks

For both the delay discounting and CRA tasks, we used ADO, which is a ML method originated from active learning[41] to optimize experimental variables, in real-time every time participants completed the tasks. We used uniform prior distributions and grid-based parameter estimation to update prior distributions of model parameters (from standard cognitive models of these tasks; see below) into posterior distributions, based on Bayes' rule. We used a Python library called ADOpy[42].

Choice under risk and ambiguity (CRA) task[36]

We used an ADO-powered CRA task to evaluate responses to risk and ambiguity, with known and unknown (ambiguous) reward probabilities (**Figure 1B**). Initially (in 2019), the CRA consisted of 60 trials (N=22), but analysis showed 30 trials were sufficient to estimate model parameters (**Figure S2**), so the number was reduced for subsequent data collection. We modeled behavior using a modified utility model, as in prior studies[36], where

the utility (U) of each option was based on reward probability (p), reward amount (R), ambiguity (A), and individual subject- (and day-) specific risk tolerance (α) and ambiguity tolerance (β), as follows.

$$U_{option} = [p - \beta(\frac{A}{2})] * R^{\alpha} \quad (1)$$

The probability of choosing the ambiguous option (Pr_{Var}) was computed by comparing the utilities of fixed-probability (U_{Fix}) and variable (U_{Var}) options.

$$Pr_{Var} = \frac{1}{1+\exp[-\gamma(U_{Var}-U_{Fix})]} \quad (2)$$

A risk tolerance parameter (α) < 1 indicates risk aversion, α > 1 indicates risk seeking, and α = 1 risk neutrality. Similarly, an ambiguity tolerance parameter (β) > 0 indicates ambiguity aversion, β < 0 indicates ambiguity tolerance (bearing with the unknown probability), and β = 0 ambiguity neutrality. For ease of interpretation, we report -β, with higher -β parameters indicating greater ambiguity tolerance. A third parameter γ captured choice stochasticity. See Supplementary materials for details.

Delay discounting task[32]

We used the 20-trial delay discounting task powered by ADO, shown to robustly estimate discount rates in our prior work (Ahn et al., 2020[38]). In each trial, participants chose between a larger-later (LL) and smaller-sooner (SS) monetary reward, with random positioning on the screen (**Figure 1C**).

Using the hyperbolic model (**Equation 3**)[43], we estimated the delay discounting rate (k), log-transformed to log(k) to address skewness in the distribution of k values. Larger log(k) values indicate greater temporal impulsivity. Subjective value (V) of each option was calculated based on reward (R) and delay (T), with Pr (LL) as the probability of choosing the LL option, and τ as the inverse temperature reflecting choice sensitivity.

$$V = R * \frac{1}{1+kT} \quad (3)$$

$$Pr_{LL} = \frac{1}{1+\exp[-\tau(V_{LL}-V_{SS})]}$$

Short-term (day-to-day) prediction of smoking behaviors

To identify factors that can predict proximal (short-term) smoking behavior, we conducted a time-lagged analysis using a linear mixed-effect model (*lme* package in R[44]). Independent variables included task parameters (log(k), α, and -β) and the self-reported psychological states (anxiety, craving, depression, stress, and mood) from the current day (t) to predict cigarettes smoked on the next day (t+1). *Day* (i.e., elapsed days at the clinic) was added as a fixed effect to account for the non-linear decline in cigarette use over time (**Figure 3B**), and between-subject variability was modeled as a random effect. Model quality was assessed using 3-fold cross-validation which was repeated 100 times to choose the best model with the smallest mean squared error in the test set.

Long-term (after treatment) prediction of smoking cessation

To predict long-term smoking cessation after treatment, we ran penalized logistic regression with 10-fold cross validation (*easyml package in* R). Predictors included survey responses, model parameters (log(k), α, and -β), age, sex, smoking duration, and weekly

clinic attendance. A marginal correlation was observed between smoking history and daily data compliance (r=0.2, p=0.08).

Participants were grouped by end-of-treatment smoking status: the “quit group” (4 weeks of self-reported abstinence and post-clinic exhaled CO ≤ 5ppm) and the “failed group”. To examine the minimum data required to predict status, we tested models using different data windows (e.g., first week vs. all available weeks; **Table S1**). In these models, we considered both mean levels and day-to-day variability of the predictive variables, quantified as root mean square of successive differences (RMSSD) for both task and survey responses (*EMAtools* package in R[45]).

Results

Participants characteristics

A total of 79 participants (25.64 years of age on average, 83% males) were included in the final analysis. The quit and failed groups did not significantly differ in demographic and baseline (pre-clinic) smoking-related variables, except for smoking duration. In addition, they differed in clinic participation (**Table 1**). Thus, we included these two variables along with demographic variables (i.e., age and sex) in the analysis predicting smoking cessation status.

Characteristic	**Failed**, N = 53[1]	**Quit**, N = 26[1]	**p-value**[2]
Age	25.64 (3.76)	26.88 (3.76)	0.2
Sex	44 (83%)	22 (85%)	>0.9
Smoking duration	4.40 (3.82)	7.77 (4.25)	0.001
CO (ppm) screening	4.00 (3.70)	3.46 (2.72)	0.5
CO (ppm) pre-clinic	3.91 (3.26)	3.46 (2.82)	0.6
CO (ppm) post-clinic	4.32 (3.43)	1.92 (0.98)	<0.001
Clinic participation (%)	58.18 (28.61)	71.15 (25.63)	0.061
FTND	1.34 (1.01)	0.94 (0.80)	0.10
App participation (%)	74.81 (23.14)	80.33 (21.53)	0.2

[1] Mean (SD); n (%)

[2] Wilcoxon rank sum test; Fisher’s exact test

Table 1. Demographic variables for the quit vs. failed smoking cessation groups

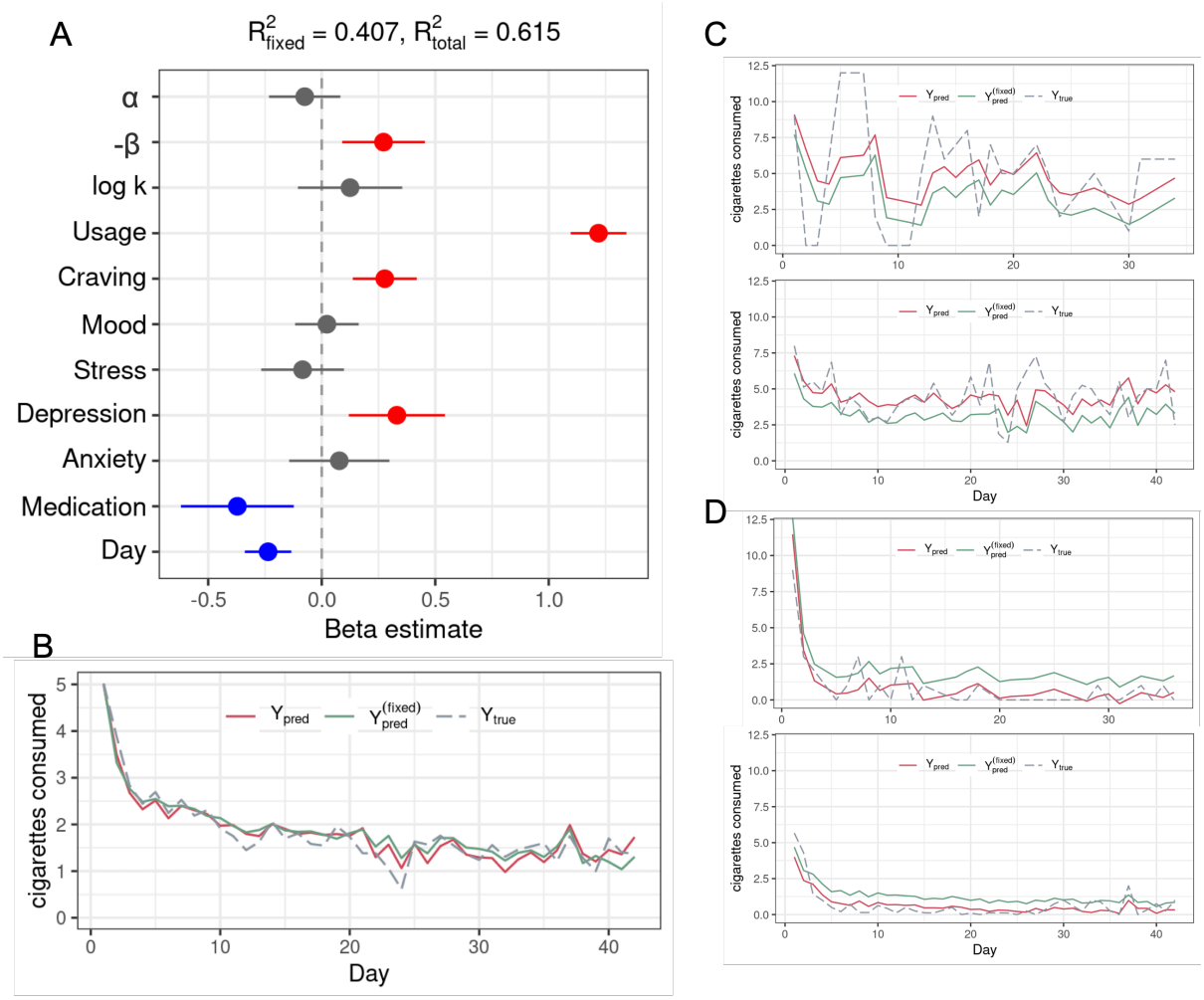

Figure 3. (A) Coefficient plot of the winning time-lagged prediction model predicting next-day number of cigarettes smoked from current day self-report and task-related variables (the last model [#29] in **Table S2**). Colored dots indicate variables with statistically significant coefficients. Error bars indicate 95% confidence interval. **(B)** Model predictions and actual cigarette consumption over time. The plot compares the observed cigarette consumption (Y_{true}) with the predicted values from a mixed-effects model (Y_{pred}) and its fixed-effects component (Y_{pred}^{fixed}). It suggests that the model is not only capable of accounting for day-to-day variations but also follows broader patterns of reduction in cigarette usage throughout the multiple days. This similarity underscores the model's utility for understanding smoking behavior dynamics, particularly for predicting future consumption based on prior variables. (**C**) Predicted and true cigarette consumption for a sample individual (upper) and for 10 individuals (lower) with a high variability (**D**) Predicted and true cigarette consumption for a sample individual (upper) and for 10 individuals (lower) with a low variability.

Short-term (day-to-day) prediction of smoking behaviors

For the short-term prediction of smoking behavior, we aimed to identify daily computational and psychological markers that could dynamically inform treatment adjustments to reduce relapse risk and enhance immediate outcomes. A time-lagged regression model that incorporates both computational markers and survey variables achieved the best accuracy compared to other models (**Table S2**). The results showed that

number of cigarettes smoked, craving for smoking, and depression level on the current day positively predict the number of cigarettes smoked on the next day (**Figure 3A**). Medication intake, by contrast, was associated with decreased smoking amount on the next day.

We found a significant contribution of ambiguity tolerance (-β) in predicting increased smoking amount on the next day, with bigger effects than the other model parameters (log(k) and α). A larger ambiguity tolerance (-β) parameter indicates stronger ambiguity tolerance, linked to increased smoking the next day. This suggests individuals more comfortable with uncertainty may be more willing to smoke despite the unknown risk for relapse and treatment failure, consistent with the previous finding[19]. This effect remained the same when we controlled for medication effects (**Table S2**). Even after controlling for the primary variance-driving factor of prior-day cigarette usage, both the ambiguity tolerance parameter and craving remained significant positive predictors in the model (**Figure S3**). This outcome suggests that these factors contribute uniquely to cigarette consumption variability independent of prior-day usage effects, which underscores the robustness of the result. Specifically, the model predicted well individuals with both high and low variability in their cigarette consumption (**Figure 3C, D**), demonstrating its potential to capture daily fluctuations in smoking behaviors. The results support short-term treatments targeting predictive factors, such as managing cravings and improving tolerance for uncertainty, to promote more consistent progress toward cessation.

Predicting smoking cessation after treatment

For the long-term prediction of smoking cessation, we aimed to identify and evaluate the efficiency of ADO-powered computational markers based on predictive accuracy. The top model (Model K, AUC=0.83, **Table S3**) used data from the full study period (5-6 weeks) where survey responses played a significant role. Models based solely on surveys achieved AUCs of 0.79 and 0.80 (Model G and Model H). Responses closer to the end of treatment were the most predictive, reflecting changes related to cessation outcomes. Models with more data points from a larger temporal window (i.e. all weeks) and more frequently sampled data (i.e., multiple days) performed better (**Table S3**), and this trend held even after controlling for the number of datapoints (Model N, AUC=0.82).

Key predictors of cessation success included lower discounting rates (log(k)), lower craving and stress, a longer smoking history, and greater treatment engagement (**Figure 4**). These findings align with prior research on impulsivity as a strong relapse factor[34,46]. Additionally, a longer smoking history and greater engagement in treatment sessions were positively associated with successful cessation, potentially reflecting increased motivation to quit among long-term smokers.

Next, we tested if we could achieve predictive accuracy with a shorter temporal window. In particular, data from the first week or two, as they flag at-risk individuals with more targeted interventions early in treatment with the goal of obtaining a higher probability of success at the end of treatment. A model using only the first week of task data (Model B, AUC=0.74) performed similarly to models based on survey data (Model F, AUC=0.73) or both task and survey data (Model J, AUC=0.76). Extending data collection beyond the first week (Model C, AUC=0.74) or adding more data within a shorter timeframe (Model D, AUC=0.73) did not improve prediction further. This outcome suggests that task-based computational markers from the initial week of treatment can predict outcomes effectively, especially when extensive data collection is not feasible. While a broader temporal window

improves prediction as a rule of thumb, we show that computational markers driven from a limited data still provide practical insights that can be leveraged in treatment programs.

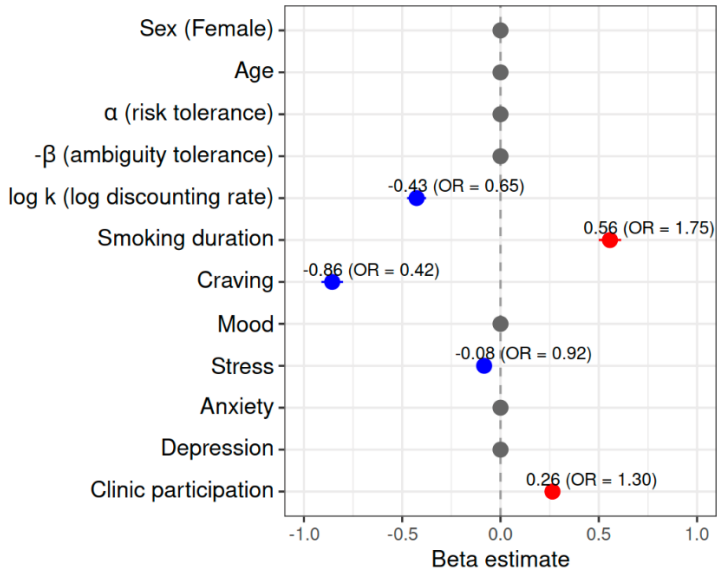

Figure 4. Results of linear logistic regression predicting the likelihood of successful smoking cessation following clinic. The labels on the left represent the input variables, for which the mean values collected during the first week were included as predictors in the model (Model J). A smaller discounting rate (k), associated with lower impulsivity, craving, and stress levels, along with a longer history of smoking and active participation in the clinic, were predictive of successful treatment outcomes. OR=Odds Ratio.

Discussion

NUD is a chronic disorder with excessive relapse rates, highlighting the need to identify dynamic predictors of smoking behavior for both short- and long-term outcomes. Theoretical models and initial empirical findings from other substance use disorders suggest that frequent sampling is needed to capture the temporal dynamics of latent neurocognitive processes in addiction. However, these approaches have not been applied to smoking behaviors, and no studies have achieved the resolution necessary to track these dynamics effectively at clinically relevant, daily timescales. Traditional methods, such as EMA—based solely on survey data—or computational modeling requiring lengthy tasks face significant feasibility and precision challenges in clinical settings.

To address these limitations, this study combined ML methods (ADO) with task-based EMA, to efficiently collect computational markers together with survey data on a daily basis over 5-6 weeks of a smoking cessation program. This innovative approach provides a promising framework for understanding the cognitive factors influencing smoking cessation outcomes. It also underscores the utility of ADO-powered computational markers to inform personalized treatment strategies for nicotine addiction.

First, we found that daily-level data, including computational markers of delay discounting and risk/ambiguity tolerance, alongside subjective psychological responses like craving and stress, were highly predictive of daily cigarette consumption patterns. Notably,

within a smaller temporal window, ambiguity-averse individuals were more likely to reduce cigarette consumption. This aligns with prior research in other substances[19] and suggests that ambiguity-tolerant individuals may be more likely to continue to smoke as they associate it with uncertain negative outcomes, even if they don't know the precise probability of harm. Interestingly, the best model predicted both next-day smoking and overall trends in cigarette intake during treatment. This ability to capture fine-grained dynamics could aid in monitoring consumption and identifying relapse risks early.

Second, we demonstrated that computational markers, even when collected over one week, achieved predictive accuracy comparable to more extensive data and survey responses. This suggests that these behavioral markers collected during an early course, such as particularly lower impulsivity (discounting rate) can effectively predict cessation success. These insights emphasize the potential of short-term (i.e., 1 week) task-based data for early intervention, particularly in settings where longer-term data collection is challenging. This replicates prior findings on the role of delay discounting rate in predicting post-treatment smoking cessation[47,48] while expanding the literature[19] by establishing a link between ambiguity aversion and daily smoking behavior. Although ambiguity aversion has been rarely studied in treatment outcome, our results suggest that it could have significant clinical utility in guiding daily treatment strategies. The findings also underscore the importance of individual differences in smoking cessation and the effectiveness of computational approaches in addressing the large variance observed across addiction stages[49]. The ability to anticipate overall consumption trends during the early treatment period could aid in the early identification of relapse risk and guide adjustments in treatment intensity to improve long-term cessation outcomes. Importantly, the computational parameters offered unique insights into the decision-making processes driving smoking behavior, extending beyond what can be inferred from survey-based measures alone.

Limitations

Our sample mostly comprised young smokers who were screened for other substance use disorders, enhancing rigorous understanding of NUD but potentially limiting generalizability to populations with co-occurring psychiatric disorders. At the same time, this age group is particularly critical to study, as more than 50% of adult smokers initiate smoking before the age of 18, and early smoking significantly increases the risk of lifelong addiction and smoking-related diseases[50] . Future studies balancing the focus on this pivotal group with broader sampling could enhance the applicability of findings while maintaining relevance to public health priorities.

Conclusion

To our knowledge, this is the first study that combines self-report and task-based data to predict smoking behavior during treatment at this fine-grained (daily) level. The fact that the one week of data was sufficient to achieve high predictive power not only reduces the burden on further research participants but also enhances the feasibility of integrating such assessments into clinical settings. This finding is valuable given the practical constraints of participant engagement and the need to minimize dropout rates in studies involving participants with psychiatric disorders.

Together, our results underscore the potential of integrating real-time responses with ADO-powered tasks to enhance the precision of behavioral predictions. This approach is both reliable and efficient in capturing individual differences while minimizing participants'

time and cognitive burden. We provide evidence that combining EMA responses with ADO-powered task parameters is both efficient and powerful in predicting the daily smoking behaviors of active smokers and in real-world treatment settings. We hope these results offer novel insights and open possibilities for more effective and precise treatments, fostering the development of individually-tailored interventions in clinical practice.

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